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An algorithm for numerical solution of Anisimov coupled differential equation of heat transfer from electron to lattice

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Abstract

This paper proposes a way of obtaining non-equilibrium transient electron-lattice temperature of several thousands of Kelvin in semiconductor thin films by applying satisfactorily boundary conditions to Anisimov coupled differential equations .This is possible by adjusting some of the parameters in the equations and tailoring the characteristics of semiconductors to achieve an enhanced transient carrier concentration and transverse spread in energy that will enhance the performance of the free-electron laser technology.

Keywords: Increase transient Concentration, transient electron temperature, skin depth, exponential growth rate, electron-phonon coupling.

1.0 Introduction

Thermal enhancement technique involves laser pumping of electrons from valence band to conduction band and emitting those excited electrons by a delayed laser pulse in addition to those usually photoemitted from valence band to the conduction band (Milonni and Eberly, 1988 [11]; Berthod, *et al*., 2004) [4]. Hence, in order to obtain thermally enhanced photoemission using ultra short laser pulses; time resolved measurement of the electron (T_e) and lattice (T_l) temperatures has to be the focus of attention (Jensen, *et al*., 2003) [9]. To do this, Anisimov, *et al*., (1974) [1] developed a coupled nonlinear differential equation (two temperature model) of heat transfer from electron to lattice of a metal irradiated with ultra shot laser pulse incident normally on the surface of a metal. An analytical solution to the equations developed by Anisimov, *et al*., (1974) [1] is next to impossible as only approximate numerical solution and experimental results is possible as has been done. In the previous papers, appropriate boundary conditions are applied to the equations and finite difference method used to develop an algorithm for numerical solution whose results of computations and applications are obtained in Musongong, *et al*., (2006) [13] ; De and Musongong, (2007) [6] and Musongong, *et al*., (2007) [14] for intrinsic semiconductors of thickness d = 1.2, 1.1 and 0.9 µm. In this paper, we are presenting an algorithm developed for n-type extrinsic GaAs semi-conducting thin film with doping concentration Nd $=10^{21}$ cm^{-3} and thickness $d = 280A^0$ for two temperature model.

The two temperatures model was first introduced and applied to a metal by Anisimov, *et al.*, (1974) [1] and subsequently applied by Fujimoto*, et al.,* (1984) [7] to tungsten. Papadogiannis, three years later applied the same equations to tungsten metal

(Papadogiannis, *et al*., 1987) [15] while Rethfeld recently applied the same idea of two temperature model (Rethfeld *et al.*, 2002) [16] to investigate theoretically the transient evolution of the distribution function of the electron gas in a metal during and after irradiation with a subpicosecond laser pulse of moderate intensity making use of Bloch functions. Moos applied the same coupled differential equations (Moos, *et al*., 2002 [12]; Anonymous 2007) [3] to single-wall carbon nanotube bundles to determine energy transfer from electrons to lattice while Jensen, *et al*., 2003 [9] applied the coupled

differential equations to the measurement and analysis of thermal photoemission from a dispenser (coated with metal of low work function) free-electron laser cathode. He discovered that photocathodes for free-electron laser are required to produce nano-Coulomb pulses in picosecond time scale with demonstrable reliability, lifetime and efficiency. Low work function coatings on semiconductors photocathodes, produced by empirical techniques have excellent quantum efficiency but suffer the fact that their response times are too large. Therefore a great deal of heat energy will be dumped into the crystal (space charge) altering their operations and leading to nonlinear performance. In general, photocathodes are often preferred to thermionic cathodes which consist of a metal with relatively low work function that is heated until electrons are emitted. This emission is explained by treating the free electrons in the metal as a Fermi-Dirac gas (Clendenin *et al*., 1999) [5]. Thermionic cathodes are characterized by low life time, high emittance, low current density, high space charge, and non repeatability (Anonymous, 2006) [3]. Thermionic cathodes sources have been used in the past for free-electron laser have had the problem of not being switched on the picosecond time scale, and the resultant emittance of the electron beam is too large to allow for lasing at desired wavelengths (Jensen *et al*., 2003) [9].

2.0 Theoretical model

The coupled nonlinear differential equations for the two temperature model are

$$\frac{C_e \partial T_e}{\partial t} = K_t \frac{\partial^2 T_e}{\partial t^2} - g(T_e - T_l) + A'_{(z,t)} \tag{2.1}$$

Since the lattice receives energy from electrons through electron phonon coupling g of both z = 0 and z > 0, then

$$C_l \frac{\partial T_l}{\partial t} = g(T_e - T_l) \tag{2.2}$$

is valid. Part of the energy is transferred to the lattice through the term $g(T_e - T_l)$. whereas radiation can take place through motion. The electron-phonon coupling factor g is given as

$$g = \frac{\pi^2 m n_e V_s^2}{6\tau_{ep} T_l} \tag{2.3}$$

where m is the effective mass of the electrons or holes, n_e is the electronic concentration and V_s is the velocity of sound in the metal and τ_{ep} is the relaxation time given by the expression

$$\frac{1}{\tau_{ep}} = aT_l + bT_l^3 \tag{2.4}$$

for any material, while a and b are constants and determined experimentally.

$A'(z,t)$ represents the source term, which is actually the z-gradient of the incident laser pulse probe intensity and R being the reflectivity at the surface of the material thin film at time t. Both C_e and C_l are functions of $t(i)$ and $z(j)$. C_e and C_l are the electronic specific heat capacity per unit volume and lattice specific heat respectively. K_t represents the thermal conductivity of the material ($Kt = 0.81\, W/cmK$ for GaAs thin films). For a given thickness d, relaxation time τ_{ep}, and gradient of the laser intensity $A\ (z,t)$ we apply numerically the finite difference method for the solution if $A'(z,t)$ is known explicitly.

3.0 The Equation of Incident Intensity (Source term)

Consider a very short incremental interval of time Δt with the time T. If we let $p(t)\Delta t$ to be the probability of ejecting an electron from the surface in a time interval Δt, the $p(t)\Delta t$ is given by

$$p(t)\Delta t = \alpha I(t)\Delta t \qquad (3.1$$

where $I(t)$ is the incident intensity average over a few optical periods and α is a constant depending on the nature of the detector (density of atoms, size of exposed surface, etc). The time interval Δt is taken to

be so short that the probability of ejecting more than one electron during this time is completely negligible. Δt is chosen not to be an intrinsic parameter of experiment but merely a theoretical construct, so that we can make it as small as possible. Then, $P_n(t)$ is defined to be the probability of *n* photons incident on the surface at time $0 \le t \le T$. We conveniently choose $P_n(t+\Delta t)$ where Δt is defined above so that there will be two mutually exclusive ways of getting *n* photons in the time interval $t+\Delta t$. We get $n-1$ photons in the time interval *t* and *1* more in the interval from *t* to $t+\Delta t$ so that its probability is given as

$P_{n-1}(t)p(t)\Delta t = (prob.\ of\ \ n-1\ photon\ in\ time\ t)\times(prob.\ of\ 1\ photon\ \ in\ time\ \Delta t)$ (3.2) The other alternative is that we get *n* photons in the time *t* and more in the interval from *t* to $t+\Delta t$, i.e.

$$P_n(t)[1-p(t)\Delta t] = [\text{prob. of } n \text{ photons in time } t]\times[\text{prob. of no photon in time } \Delta t] \qquad (3.3)$$

Since both cases we want *n* photons, then adding (3.2) and (3.3) we have

$$P_n(t+\Delta t) = P_{n-1}(t)p(t)\Delta t + P_n(t)[1-p(t)\Delta t] \qquad (3.4)$$

Rearranging (3.4) we obtained

$$\frac{P_n(t+\Delta t)-P_n(t)}{\Delta t} = p(t)[P_{n-1}(t)-P_n(t)] \qquad (3.5)$$

Since Δt is at our disposal to make it small as possible we let it become a derivative of $P_n(t)$ so that the left hand side of (3.5) becomes

$$\frac{P_n(t+\Delta t)-P_n(t)}{\Delta t} \approx \lim_{\Delta t \to 0} \frac{P_n(t+\Delta t)-P_n(t)}{\Delta t} = \frac{dP_n(t)}{dt} \qquad (3.6)$$

Therefore equation (3.5) becomes

$$\frac{dP_n(t)}{dt} = p(t)[P_{n-1}(t)-P_n(t)] \qquad (3.7)$$

Using equation (3.1) for *P(t)* we obtain

$$\frac{dP_n}{dt} = \alpha I(t)[P_{n-1}(t)-P_n(t)] \qquad (3.8)$$

Solving (3.8) we obtained

$$\begin{aligned} \frac{dP_n}{dt} &= \frac{1}{n!}X(t)^n \frac{d}{dt}\left(e^{-X(t)}\right) + \frac{1}{n!}e^{-X(t)}\frac{d}{dt}X(t)^n \\ &= \frac{1}{n!}X(t)^n\left(-\frac{dX}{dt}e^{-X(t)}\right) + \frac{1}{n!}e^{-X(t)}\left(nX(t)^{n-1}\frac{dX}{dt}\right) \\ &= \frac{dX}{dt}\left(\frac{[Xt]^{n-1}}{(n-1)!}e^{-X(t)} - \frac{[X(t)]^n}{n!}e^{-X(t)}\right) = \frac{dX}{dt}[P_{n-1}(t)-P_n(t)] \end{aligned} \qquad (3.9)$$

Hence $$P_n(t) = \frac{1}{n!}X(t)^n e^{-X(t)} \qquad (3.10)$$

which is an exact solution of (3.8) and

$$\frac{dX(t)}{dt} = \alpha\frac{d}{dt}\int_0^t I(t')dt' = \alpha I(t) \qquad (3.11)$$

Equation (3.9) is equivalently written as

$$P_n(T) = \frac{[XT]^n}{n!}\exp^{-X(t)} \qquad (3.12)$$

where $$X(T)=\alpha\int_0^T I(t)dt \tag{3.13}$$

Equation (3.13) is an elegant solution of the integral but the interval of time goes from zero to T. We are dealing with large interval of time not starting from zero hence we modified equation (3.13) for interval of time t to $t + T$ *as*

$$X(t,T)=\alpha\int_t^{t+T} I(t)dt' \tag{3.14}$$

or $$X(t,T)=\alpha T\bar{I}(t,T) \tag{3.15}$$

where $$\bar{I}(t,T)=\frac{1}{T}\int_t^{t+T} I(t')dt' \tag{3.16}$$

is the average incident intensity during the time interval from t to $t + T$ .Then equation (3.12) becomes

$$P_n(t,T)=\frac{1}{n!}[X(t,T)]^n\exp[-X(t,T)] \tag{3.17}$$

For a two dimensional thin film of incident laser pulses, equation (3.17) is modified as we took into consideration the duration of the pulses and the depth of the penetration on the surface of the thin film. Hence equation (3.17) is equivalently written as

$$A(r,t)=A_0\exp\left[-\left(\frac{t-\tau}{2\tau}\right)^2 4\ln 2\right] \tag{3.18}$$

for a Gaussian surface.

Therefore: $$A(0,t)=A_0(1-R)\exp\left(-\frac{1}{4}\left\{\frac{t-\tau}{\tau}\right\}^2\ln 2\right) \text{ at } z=0 \tag{3.19}$$

4.0 Application of boundary conditions

The boundary conditions that exist at the surface are:

$$-K_t\frac{\partial T_e}{\partial z}=A_0(1-R)\exp(-\frac{z}{\delta})\exp\left(-\frac{1}{4}\left\{\frac{t-\tau}{\tau}\right\}^2\right)\ln 2 \tag{4.1}$$

for Gaussian pulse.

$$-K_t\frac{\partial T_e}{\partial t}=A_0(1-R) \tag{4.2}$$

for square pulse for $0 < t \le \tau$. For a given thickness *d,* relaxation time τ_{ep}, δ the skin depth and gradient of the laser intensity *A (z,t)* we apply numerically the finite difference method for the solution. We took N = 1000 being the divisions of both the time τ (the laser pulse width) = 1 nanosecond and the thickness *d*. We calculated the values of $T_e\ (i,j)$ and $T_l(i,j)$ and obtained the average temperature $\langle T_e(i)\rangle$ and $\langle T_l(i)\rangle$ respectively for intrinsic Gallium Arsenide (GaAs) thin film. Here we have assumed $\frac{1}{\tau_{ep}T_l}=1$ for simplifications. We took $d = 280\ A^0$ and $100\ A^0$ respectively for different thicknesses and peak pulses of 0.01, 0.1, 5, 10 and 350 MW/cm^2 respectively. We compared our results with the well known result of Jensen, *et al*. (2003) and Fujimoto, *et al.* (1984) to cross-check our method of calculations. We also extended the divisions from 1000 to 5000 or more for a better result.

For a two dimensional thin film with pump laser incident along the *z*-direction where $t = i$, $z = j$ as running index we have

$$-k_t \frac{\partial T_e}{\partial z} = \frac{k_t [T_e(i, j+1) - T_e(i, j)]}{\Delta z} = A_O$$

$$\forall \; z = 0 \qquad (4.3)$$

Equations (4.3) are boundary conditions and

$$\frac{C_e \partial T_e}{\partial t} = \frac{C_e[T_e(i+1, j) - T_e(i, j)]}{\Delta t} \qquad (4.4)$$

and
$$K_t \frac{\partial^2 T_e}{\partial z^2} = \frac{K_t[T_e(i, j+2) - 2T_e(i, j+1) + T_e(i, j)]}{\Delta z^2} \qquad (4.5)$$

$$g(T_e - T_l) = g[T_e(i, j) - T_l(i, j)] \qquad (4.6)$$

where
$$C_l \frac{\partial T_l}{\partial t} = \frac{C_l[T_l(i+1, j) - T_l(i, j)]}{\Delta t} \qquad (4.7)$$

Equations (4.4 - 4.7) cannot be solved directly. Applying the boundary conditions (4.4) and taking $i = 0 - 999, \quad j = 0 - 999$, we solve the equations simultaneously. We modified the boundary condition by letting

$$T_e(0, j) = T_l(0, j) = 300k. \qquad (4.8)$$

also,
$$T_e(0,0) = T_l(0,0) = 300k. \qquad (4.9)$$

We are interested in averages. In this case we consider the length of the pulse width. Since this is very small, it is clear that this can be done in one dimensional where the temperature distribution at the surface is determined by the intensity within the laser beam. Then, integrating equation (2.1) we have

$$\int C_e \frac{\partial T_e}{\partial t} dz = \int K_t \frac{\partial^2 T_e}{\partial z^2} dz - \int g(T_e - T_l) dz + A(t) \qquad (4.10)$$

where $A(t)$ is the source term and taking the integrals in (4.10) term by term we have

$$\int K_t \frac{\partial^2 T_e}{\partial z^2} dz = \int \frac{K_t[T_e(i, j+2) - 2T_e(i, j+1) + T_e(i, j)]dz}{\Delta z^2}$$

$$= \sum_i \frac{K_t[T_e(i, j+2) - 2T_e(i, j+1) + T_e(i, j)]\frac{d}{N}}{\Delta z^2} \qquad (4.11)$$

$$= K_t \sum_j \frac{[T_e(i, j+2) - 2T_e(i, j+1) + T_e(i, j)]\frac{d}{N}}{\left(d/N\right)^2} = \frac{N}{d}[T_e(i,2) - 2T_e(i,1) + \sum T_e(i, j)]K_t$$

for $j = 0$ where d is the thickness of the thick film and
$$\Delta z^2 = \left(\frac{d}{N}\right)^2 \qquad (4.12)$$

where N=1000. But
$$\langle T_e(i) \rangle = \frac{1}{N}[T_e(i,0) + T_e(i,1) + T_e(i,2) + \cdots T_e(i,999)] \qquad (4.13)$$

where $\langle T_e(i) \rangle$ is the mean electron temperature and the summation is over *j*. Hence,

$$\frac{1}{N}\sum_j T_e(i, j+2) = [T_e(i,2) + T_e(i,3) + \ldots T_e(i,99) + T_e(i,1000) + T_e(i,1001)]/N$$

$$= \left\langle \langle T_e(i) \rangle + \frac{1}{N}[T_e(i,1000) + T_e(i,1001) - T_e(i,0) - T_e(i,1)] \right\rangle \qquad (4.14)$$

also

$$\sum_j T_e(i, j+1) = T_e(i,1) + T_e(i,2) + T_e(i,3) + \cdots T_e(i,999) + T_e(i,1000)$$
$$= N\langle T_e(i)\rangle + [T_e(i,1000) - T_e(i,0)] \tag{4.15}$$

and

$$\sum_j T_e(i, j) = T_e(i,0) + T_e(i,1) + T_e(i,2) + \cdots T_e(i,999)$$
$$= N\langle T_e(i)\rangle \tag{4.16}$$

Hence,

$$\int K_t \frac{\partial^2 T_e}{\partial z^2} = \frac{K_t N}{d}\left[\langle T_e(i)\rangle + \{T_e(i,1000) + T_e(i,1001) - T_e(i,0) - T_e(i,1)\}\right]$$
$$-2\langle T_e(i)\rangle - 2T_e(i,1000) + 2T_e(i,0) + \langle T_e(i)\rangle = K_t \frac{N}{d}[T_e(i,0) - T_e(i,1)] \tag{4.17}$$

also,

$$\int C_e \frac{\partial T_e}{\partial t} dz = C_e \frac{\left[\sum_j T_e(i+1, j) - T_e(i, j)\right]\frac{d}{N}}{\Delta t} = C_e d \frac{\left[\frac{1}{N}\sum T_e(i+1, j) - T_e(i, j)\right]}{\Delta t} \tag{4.18}$$

and
$$C_l \int \frac{\partial T_l dz}{\partial t} = C_l d \frac{[\langle T_l(i+1)\rangle - \langle T_l(i)\rangle]}{\Delta t} \tag{4.19}$$

and
$$\int g[T_e - T_l]dz = gd[\langle T_e(i)\rangle - \langle T_l(i)\rangle] \tag{4.20}$$

Bringing (4.18), (4.19) and (4.20) together we obtained

$$C_e \frac{d[\langle T_e(i+1)\rangle - \langle T_e(i)\rangle]}{\Delta t} = \frac{K_t N}{d}[T_e(i,0) - T_e(i,1)] - gd[\langle T_e(i)\rangle - \langle T_l(i)\rangle] \tag{4.21}$$

and
$$C_l d \frac{[\langle T_l(i+1)\rangle - \langle T_l(i)\rangle]}{\Delta t} = gd[\langle T_e\rangle(i) - \langle T_l(i)\rangle] \tag{4.22}$$

The boundary conditions are applied as:-

$$-K_t \frac{\partial T_e}{\partial z} = A_0 \exp\left[-\left(\frac{t-\tau}{2\tau}\right)^2 \ln 2\right] \tag{4.23}$$

$$-K_t \frac{[T_e(i, j+1) - T_e(i, j)]}{\Delta z} = A_0 \exp\left[-\frac{1}{4}\left(\frac{t-\tau}{\tau}\right)^2 \ln 2\right] \tag{4.24}$$

for Gaussian pulse. At the surface $j = 0$, or

$$-\frac{Kt[T_e(i,1 - T_e(i,0))]}{\Delta z} = A_0 \exp\left[-\left(\frac{t-\tau}{2\tau}\right)^2 \ln 2\right] \tag{4.25}$$

$$\Rightarrow \quad T_e(i,0) - Te(i,1) = \frac{A_0}{K_t}\frac{d}{N}\exp\left[-\left(\frac{t-\tau}{2\tau}\right)^2 \ln 2\right] \tag{4.26}$$

and $$\left\langle T_e(i+1)\right\rangle = \frac{A_0 \Delta t \exp\left[-\left(\frac{t-\tau}{2\tau}\right)^2 \ln 2\right]}{C_e d} - \frac{g\Delta t}{C_e}\left[\left\langle T_e(i)\right\rangle - \left\langle T_l(i-1)\right\rangle\right] + \left\langle T_e(i)\right\rangle \quad (4.27)$$

and $$\left\langle T_l(i+1)\right\rangle = \frac{g\Delta t}{C_l}\left[\left\langle T_e(i)\right\rangle - \left\langle T_l(i-1)\right\rangle\right] + \left\langle T_l(i)\right\rangle \quad (4.28)$$

We have set in the method of finite difference and adjust the running integers to suit the equations. The calculations of $<T_e(t)>$ is shown in figure 1 for GaAs semi-conducting thin film material. In the finite difference method an algorithm for the solution of differential equation, $C_e(T_e)$ has to vary as shown in Musongong, *et al*., (2007) [14]. Hence

$$C(T_e(i,j))^* = \frac{\sqrt{2}}{\hbar^3 \pi^2}\left[\frac{15}{8}\pi^{1/2} K_B^{5/2} T_e^{3/2}(i,j) + \frac{3\pi^{1/2}}{8} K_B^{3/2} T_e^{1/2}(i,j)\varepsilon_g\right] \left(m_e^{*\frac{3}{2}} + m_h^{*\frac{3}{2}}\right)\exp\left(-\frac{\varepsilon_g}{2K_B T_e(i,j)}\right) \quad (4.29)$$

where $C(T_e(i,j)$ is a function of transient electron temperature $T_e(i,j)$. We incorporate (4.28) into (4.27) to obtain:

$$\left\langle T_e(i+1)\right\rangle = \frac{A_0 \Delta t \exp\left[-\left(\frac{t-\tau}{2\tau}\right)^2 \ln 2\right]}{C_e\left\langle T_e(i)\right\rangle^{**} d} - \frac{g\Delta t}{C_e\left\langle T_e(i)\right\rangle^{**}}\left[\left\langle T_e(i)\right\rangle - \left\langle T_l(i-1)\right\rangle\right] + \left\langle T_e(i)\right\rangle \quad (4.30)$$

where $C_e(i)^{**} = \sum C_e(\left\langle T_e(i)\right\rangle)$, and

$$\left\langle T_l(i+1)\right\rangle = \frac{g\Delta t}{C_l(i)}\left[\left\langle T_e(i)\right\rangle - \left\langle T_l(i-1)\right\rangle\right] + \left\langle T_l(i)\right\rangle \quad (4.31)$$

where the sum is over j and $n_e(T_e(i))$ incorporated in the expression for g in equation (2.3). We have to develop an equation incorporating $n_e(T_e(i))$.

When an electromagnetic field is incident on a semiconductor sample, energy is supplied to the free carriers at the rate $\sigma(A)A'(z,t)$, where σ is the intensity-independent free carriers absorption cross section, and $A(z,t)$ represents the intensity inside the sample. A steady state is attained when the average rate of energy gained from the field equals the average rate of energy lost by the emission of phonons $\left\langle \frac{d\varepsilon}{dt}\right\rangle$.That is,

$$\sigma(A)A'(z,t) + \left\langle \frac{d\varepsilon}{dt}\right\rangle = 0 \quad (4.32)$$

At low light intensity, free electrons occupy states near the conduction band in minimum number while the valence band is filled. At high light intensities, the electron temperature becomes much greater than the lattice temperature. This modification in the carrier distribution introduces intensity dependence in the free carrier absorption cross-section. For the indirect intra conduction and intra valence band transition, the excitation rates are assumed to depend only on the density of the final states to which the free carriers can be excited by the absorption of a single photon. Thus, the indirect free carrier absorption depends on the electron temperature and increases as the intensity of the incident light increases.

The indirect free carrier cross-section for photon energy $\hbar\omega$ is given by:

$$\sigma(\omega)=\sum_{k}\sigma\{\varepsilon(k),\omega\}f\{\varepsilon(k),T_e\} \tag{4.33}$$

where $f\{\varepsilon(k),T_e\}$ is the distribution function for a state with energy ε and carrier temperature T_e with $\sigma(\omega)$ as the cross-section. It is assumed that $\sigma(\varepsilon,\omega)$ is proportional to the density of electronic states at $\varepsilon+\hbar\omega$ where the constant of proportionality is determined by requiring that at low light intensities $\sigma(\omega)$ is experimentally determined. From equation (4.33), to determine the carrier temperature as a function of the light intensity, we require the rate of energy loss from the electron system to the lattice system. For a covalent semiconductor, the carrier-phonon interaction was described by James, (1983) [8], as a deformation potential. Based on the James model, the matrix element of scattering by acoustical and optical models are given by:

$$\left|M_{ac}\right|^2=\frac{\varepsilon_{ac}K_BT_l}{2V\rho\mu_l^2} \tag{4.34}$$

$$\left|M_{op}^{+}\right|^2=\frac{D^2\hbar}{2V\rho\omega_{op}}\left(N_{op}+1\right) \tag{4.35}$$

and

$$\left|M_{op}^{-}\right|^2=\frac{D^2\hbar}{2v\rho\omega_o}N_{op} \tag{4.36}$$

where $\left|M_{ac}\right|^2$ is the squared acoustic phonon scattering matrix element (summed over both absorption and emission), $\left|M_{op}^{+\,2}\right|$ is the square matrix element for optical emission and $\left|M_{op}^{-\,2}\right|$ is the squared matrix element for optical phonon absorption, ε_{ac} is the deformation potential for acoustical phonon scattering. T_l is as defined before, ρ represents the density of sample and μ_l has been taken as the sample longitudinal sound velocity, V is the volume of the sample. N_{op} represents the optical phonon Bose factor, while D is the shift of the band edge per unit relative displacement of the sub lattices. Then,

$$D=\frac{\varepsilon_{op}\omega_{op}}{\mu_l} \tag{4.37}$$

where ε_{op} represents the deformation potential for optical phonon scattering and ω_{op} is the angular frequency of the optical phonon. The average rate at which a carrier loses energy to the lattice over all possible emission and absorption processes that the carrier may undergo and this is done using the Maxwell Boltzmann distribution function. That is

$$\left\langle\frac{d\varepsilon}{dt}\right\rangle_{op}=\frac{-8(2)^{1/2}}{\pi^{\frac{1}{2}}}\frac{\varepsilon_{ac}m^{5/2}}{\hbar^4\rho}\left(K_BT_e\right)^{3/2}\left(1-\frac{T_l}{T_e}\right) \tag{4.38}$$

and

$$\left\langle\frac{d\varepsilon}{dt}\right\rangle_{op}=\frac{-(2)^{1/2}}{\pi^{1/2}}\frac{Dm^{3/2}}{\pi\hbar^2\rho}\left(K_BT_e\right)^{1/2}B\left(x_o,x_e\right) \tag{4.39}$$

where

$$B\left(x_o,x_e\right)=\frac{e^{(x_o,x_e)}-1}{e^{x_o}-1}\left(\frac{x_e}{2}\right)e^{xe/2}K_o\left({x_e}/{2}\right) \tag{4.40}$$

and

$$x_e=\frac{\hbar\omega_{op}}{K_BT_e} \tag{4.41}$$

$$x_o = \frac{\hbar \omega_{op}}{K_B T_l} \tag{4.42}$$

Also K_o is a modified Bessel function of the second kind.

For *n*-type, a direct group III and V semiconductor such as GaAs, the acoustic term is negligible and the non-polar optical scattering may be important for highly energetic carriers only. Therefore, the polar optical scattering is dominant, hence,

$$\left\langle \frac{d\varepsilon}{dt} \right\rangle_{po} = -\left(\frac{2K_B \Theta_D}{\pi M_e} \right)^{1/2} e\varepsilon_o \frac{e^{(x_o - x_e)} - 1}{e^{x_o} - 1} x_e^{1/2} e^{x_e/2} K_o\left(x_e/2 \right) \tag{4.43}$$

where
$$x_o = \frac{t_1 \omega_l}{k_B T_l} \tag{4.44}$$

$$x_e = \frac{\hbar \omega_e}{k_B T_e} \tag{4.45}$$

$\hbar$ is the normalized Planck constant and Θ_D is the Debye temperature.

In the above calculation, the carrier concentrations are considered sufficiently low to ignore any screening effects, which would reduce the interaction of the carriers with the lattice. For hot carriers, impact ionization events are energetically allowed, leading to the formation of additional electron-hole pairs. To calculate the rate of formation of non-equilibrium excess free carriers for light intensity *I*, it is necessary to first calculate the impact ionization rate for hot electron energy ε. Following Kane, (1967) [10], the impact of ionization rate for an electron with energy ε is given by:

$$\omega(\varepsilon) = A\int \rho(\varepsilon_2)\rho(\varepsilon_3)\rho(\varepsilon_4)\delta(\varepsilon - \varepsilon_2 - \varepsilon_3 - \varepsilon_4)d\varepsilon_2 d\varepsilon_3 d\varepsilon_4 \tag{4.46a}$$

where
$$A = \frac{\frac{2\pi}{\hbar}\left[|M_a|^2 + |M_b|^2 \right] - \left[\frac{M_a^* M_b + M_a M_b^*}{2} \right]}{8N_e} \tag{4.46b}$$

Here N_e represents the number of unit cells and ρ is the density of electronic states. M_a *and* M_b are the direct and exchange coulombs matrix element defined by:

$$M_a = \frac{4\pi e^2}{KV} \frac{F_{cv}(k_1, k_1')F_{ec}(k_2, k_2')}{(k_1 - k_1')^2 + L_D^{-2}} \tag{4.47}$$

and
$$M_b = \frac{4\pi e^2}{V} \frac{F_{cc}(k_1, k_2')F_{cv}(k_2, k_1')}{(k_2 - k_1')^2 + L_D^{-2}} \tag{4.48}$$

where
$$F_{nn'}(k, k') = \int \cup_n^* (k, r) \cup_n' (k', r) dr^3 \tag{4.49}$$

and $\cup_n$ is periodic part of Bloch function. L_D represents the Debye length, k_2 is the wave vector of the initial hot electron in the conduction band, k_1' is the wave vector of the additional hole in the valance band produced by impact ionization event, k_1 is the wave vector of the additional electron in the conduction band produced by impact ionization event and k_2' is the wave vector of the free electron in the conduction band after the impact ionization $\alpha(s^{-1})$. Hence

$$N_e(A) = \frac{\sum_i n_i \omega(\varepsilon_i)}{\varepsilon_i > \varepsilon_g} \tag{4.50}$$

where n_i is the free electron density in the ith energy interval.

Using the Maxwell Boltzmann distribution with electron temperature T_e, we calculate the impact ionization as a function of intensity $\alpha(A)$. That is the exponential growth rate α of the semiconductor.

Following the theory of James, we calculated the exponential growth rate as a function of intensity and electron-hole temperature as function of intensity of 10.6 and 9.6 micron wavelengths of CO_2 laser for various semi-conducting materials. We also consider the effect of thickness of the material on the exponential growth rate while being irradiated by a pulse of given time duration. Also we calculated the hot electron temperature as a function of time and depth within the material. That is

$$\alpha = \alpha(A) \qquad (4.51)$$

Then we get the electron temperature as function of intensity, as

$$T_e = T_e(A) \qquad (4.52)$$

We then combine the equations (4.51) and (4.52) to eliminate A(z,t) and obtain the exponential growth rate as a function of transient hot electron temperature. That is

$$\alpha = \alpha(T_e) \qquad (4.53)$$

Then with the help of equations (2.1) - (2.4) and (4.29 – 4.31) we calculate $\langle T_e(t)\rangle$ and also $\langle T_l(t)\rangle$ for semiconductor films of different thicknesses in the nano-second regime. Thus we get

$$T_e = T_e(t), \qquad (4.54)$$

and

$$\alpha = \alpha(t) \qquad (4.55)$$

so that

$$N_e(t) = N_{eo} \exp \int_0^t \alpha(t)dt \qquad (4.56)$$

and

$$\int \alpha(t)dt = \sum \alpha(t)\Delta t \qquad (4.57)$$

where N_e represents the density of the transient hot electrons in the conduction band and N_{eo} is the equilibrium electron density in the conduction band of the semiconductor.

5.0 Results and conclusions

The results of our calculation of the enhanced concentration of GaAs is shown in Figure 2 alongside that of non-equilibrium temperature average $\langle T_e(t)\rangle$ Figure1. These results have been obtained after a series of computer programming as shown in Appendix. It is shown in figure 1 that non-equilibrium temperature exists in semiconductor just like the metal counterpart.

Hence, the non-equilibrium signifies increase (enhancement) in the concentration in the conduction band (James, 1983) [8] of semiconductors and others.

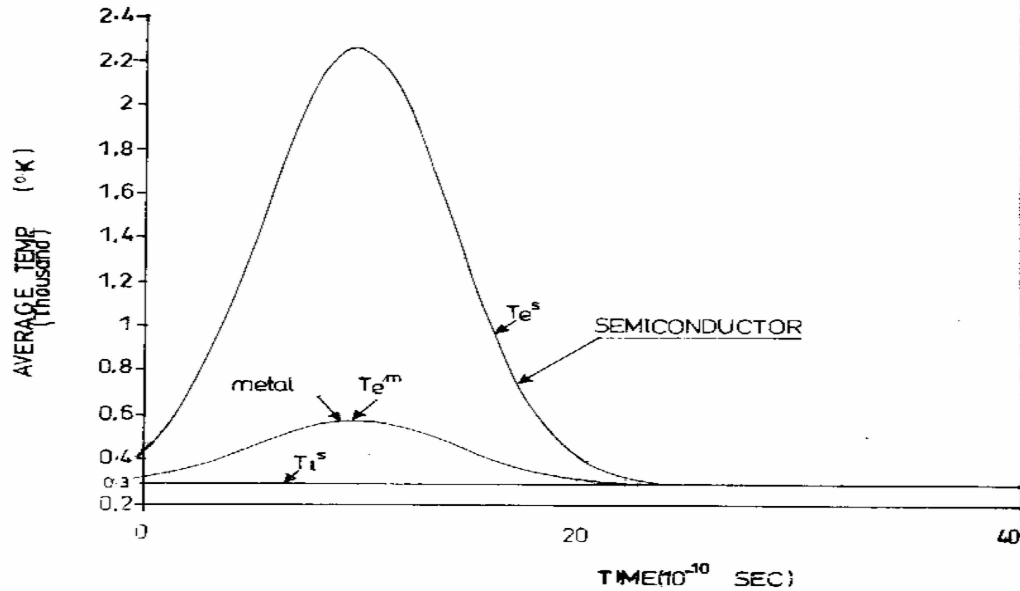

Figure. 1 . Transient electron temperature profile in GaAs semiconductor (with doping concentration, $N_d = 10^{21}$ /m^3) and tungsten metal with $\tau = 1$ns. The film thickness = 2.8×10^{-6} cm = $280\,A^0$. (It is seen that due to low electron phonon coupling in semiconductor, the electron temperature T_e is much higher than the corresponding lattice temperature T_l. The lattice temperature for metal W is the same as that of semiconductor thin film lattice temperature. $A_o = 10$ MW/cm^2).

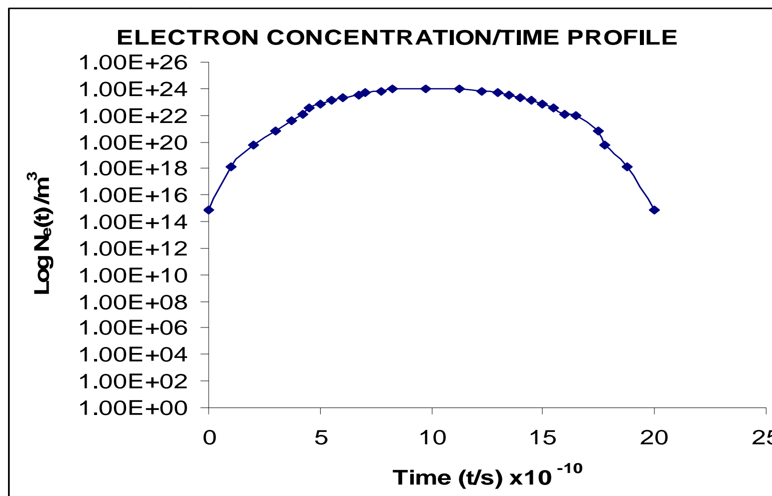

Figure 2: Transient electron concentration profile in *GaAs* irradiated with 10 MW/cm^2 and pulse width τ, = 1ns. Thin film thickness = $280A^0$.

It has been shown from Figure 2 that there is an enhancement factor of 10^8 in the concentration within 1 nanosecond at FWHM (full wave at half maximum).

APPENDIX

A computer programme for solutions.

```
Option Explicit
Public alf  As Single
Public bet As Single
Public gam As Single
```

```
Public i As Integer
Public finishI As Integer
Public t As Single
Public tau As Single
Public tFactor As Integer
Public interval As Integer
Public Te() As Single
Public Tl() As Single
Public Const fourLNtwo = 2.772588722

Option Explicit
Private Sub cmdOK_Click()
Dim rowCount As Integer
  alf = CSng(txtAlf)
  bet = CSng(txtBet)
  gam = CSng(txtGam)
  finishI = CInt(txtFinishI)
  tau = CSng(txtTau)
  tFactor = CInt(txtTFactor)
  interval = CInt(txtInterval)
  ReDim Te(finishI)
  ReDim Tl(finishI)
  Te(0) = 300
  Tl(0) = 300
 Te(1) = alf * Exp(-1 * fourLNtwo) + Te(0)
  Tl(1) = Tl(0)
  Te(finishI) = Te(0)
  Tl(finishI) = Tl(0)
  For i = 1 To finishI - 2
    t = i * 10 ^ -12 'tau / finishI
    Te(i + 1) = alf * Exp(-1 * (t / tau - 1) ^ 2 * fourLNtwo) - bet * (Te(i) - Tl(i - 1)) + Te(i)
    Tl(i + 1) = gam * (Te(i) - Tl(i - 1)) + Tl(i)
  Next i
  With FlexGrid
    .Rows = finishI \ interval + 2
    .Cols = 3
    .TextMatrix(0, 0) = "i"
    .TextMatrix(0, 1) = "Te<i>"
    .TextMatrix(0, 2) = "Tl<i>"
    rowCount = 0
    For i = 0 To finishI Step interval
      rowCount = rowCount + 1
      .TextMatrix(rowCount, 0) = i
      .TextMatrix(rowCount, 1) = Te(i)

      .TextMatrix(rowCount, 2) = Tl(i)
    Next i
  End With
End Sub
Private Sub cmdToTextFile_Click()
Dim i As Long
```

```
    Open "C:\values.txt" For Output As #1
    Print #1, "Te(i)"
    For i = 0 To finishI
        Print #1, Te(i)
    Next i
    Print #1,
    Print #1,
    Print #1, "Tl(i)"
    For i = 0 To finishI
        Print #1, Tl(i)
    Next i
    Print #1, "alpha ="; alf
    Print #1, "beta ="; bet
    Print #1, "gamma ="; gam
    Print #1, "tau ="; tau
    Close #1
End Sub.
```

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